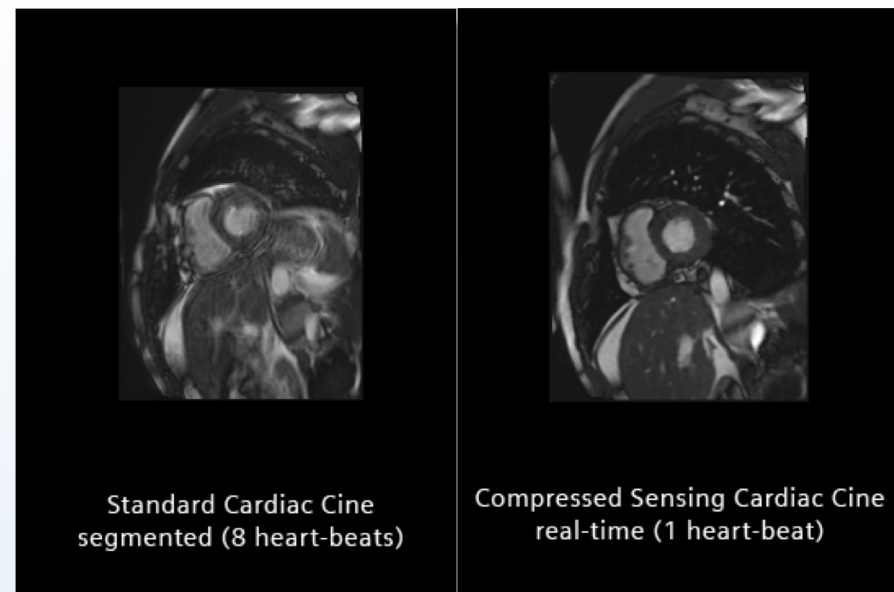


HARNESSING THE DATA REVOLUTION IN THE MATHEMATICAL AND PHYSICAL SCIENCES



BIG DATA IS CHANGING SCIENCE RESEARCH

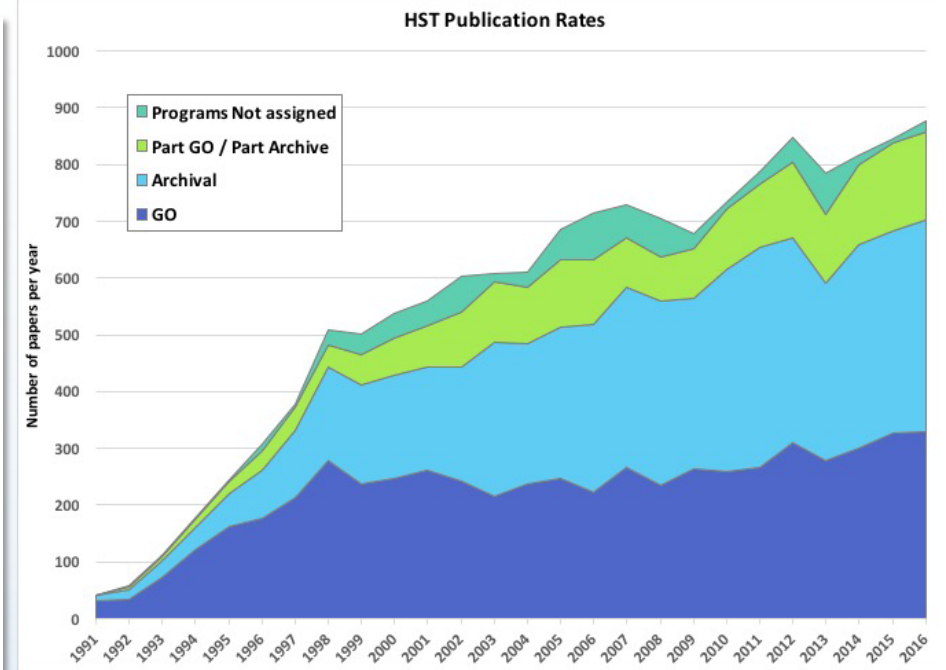
- NOVEL WAYS TO TAKE ADVANTAGE OF THE EVER GROWING BODY OF DATA
- MORE DATA LEADING TO BETTER PREDICTIONS AND DECISIONS
- MORE CONFIDENCE IN OUR MODELS AND RESULTS



A FOCUSED RESEARCH GROUP ON MULTISCALE GEOMETRIC ANALYSIS – THEORY, TOOLS, APPLICATIONS. DMS – 0140698/DONOHO (LEAD), DMS – 0140540/CANDES, DMS – 0140587/HUO, DMS – 0140623/JONES



DATA-DRIVEN ASTRONOMY



HUBBLE SPACE TELESCOPE PUBLICATION RECORD (1991-2016)

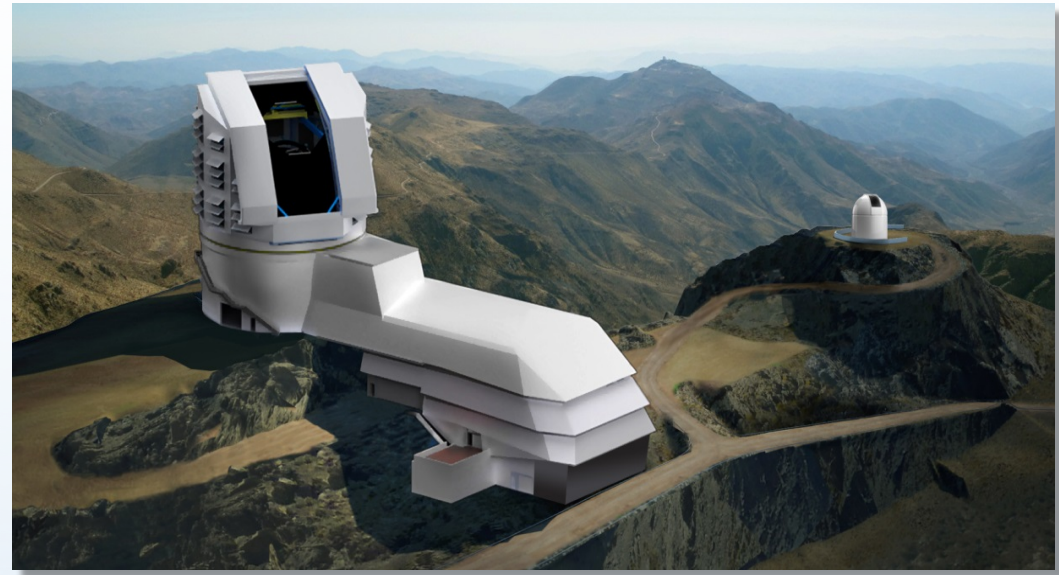
LIGHT BLUE IS RESEARCH BASED ON THE ARCHIVE

DARK BLUE IS TARGETED GUEST OBSERVERS



LARGE SYNOPTIC SURVEY TELESCOPE — *A 10-YR SURVEY OF 20 BILLION OBJECTS IN SPACE & TIME*

- VERY LARGE DATASETS ALLOW FOR:
 - PRECISION STATISTICAL ANALYSIS AND
 - AUTOMATED SEARCH FOR RARE EVENTS
- HIGH DIMENSIONALITY DATA EXPLORATION
 - AUTOMATED DISCOVERY
 - AUTOMATED DATA QUALITY ASSESSMENT
- A NEW WINDOW ON THE UNIVERSE - EXPECT THE UNEXPECTED
- TRANSFORMATIVE IMPACT OF SKY SURVEYS - CHANGE IN ASTRONOMICAL CULTURE



**SPECIALLY DESIGNED FOR SURVEYS: 15-40 TB PER NIGHT;
DATA TRANSFER CHILE->US IN 5s**

*A UNIQUE DISCOVERY ENGINE, TRANSFORMATIVE IN SCIENCE, IN EDUCATION
& OUTREACH, AND IN DATA-ENABLED SCIENCE & CYBERINFRASTRUCTURE*

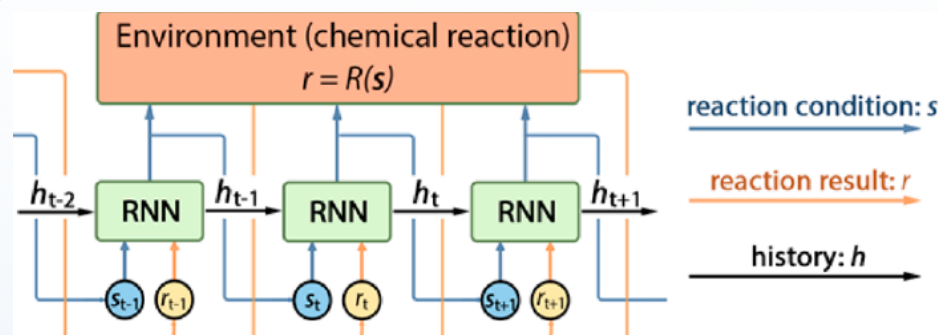


HARNESSING DATA REVOLUTION IN CHEMISTRY

DATA DRIVEN DISCOVERY SCIENCE IN CHEMISTRY (D3SC)

- CAPITALIZING ON THE DATA REVOLUTION AND PROMOTE DATA-DRIVEN DISCOVERIES TO ADVANCE FUNDAMENTAL UNDERSTANDING OF COMPLEX CHEMICAL SYSTEMS.
- USING DEEP LEARNING TO FIND ALGORITHMS FOR OPTIMIZING CHEMICAL REACTIONS (CHE-1734082, ZARE/STANFORD: D3SC:EAGER)

ACS CENT. SCI. 2017, 3, 1337–1344



DIBBS: THE LOCAL SPECTROSCOPY DATA INFRASTRUCTURE (LSDI)

- ESTABLISHING A UNIQUE COMPUTATIONAL INFRASTRUCTURE FOR SPECTROSCOPIC DATA AND CORRELATING SUCH SPECTRA WITH SPECIFIC ELECTRONIC STRUCTURE, BONDING AND LOCAL ATOMIC ENVIRONMENTS
- (NSF 1640899, KRISTIN PERSSON/UC BERKELEY, SUPPORTED BY OAC/DMR/CHE/CMMI).

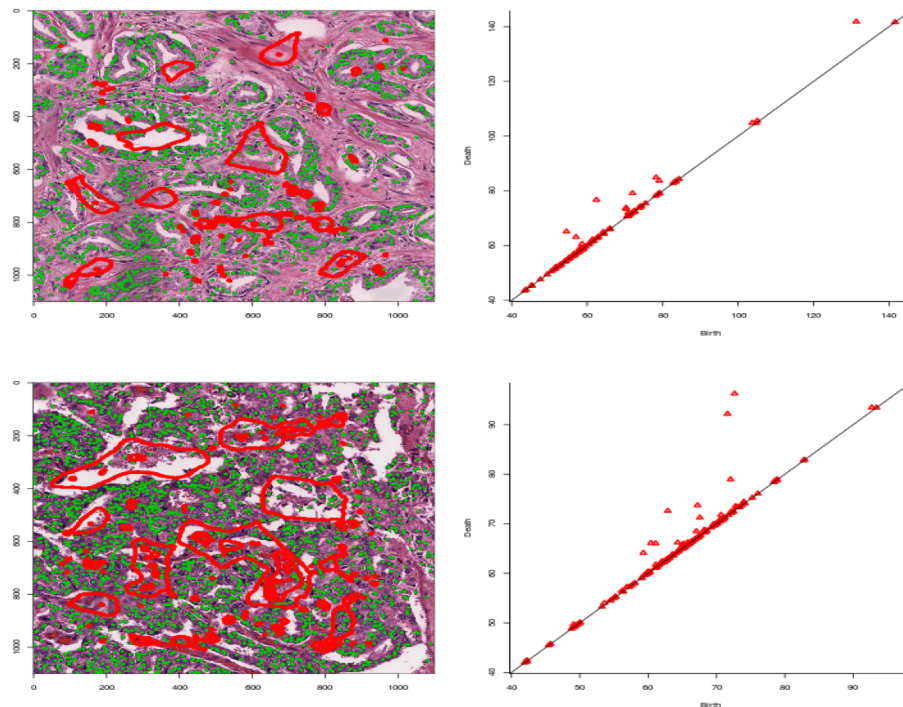


[HTTPS://DIBBS17.ORG/REPORT/POSTERS/1640899POSTER.PDF](https://dibbs17.org/report/posters/1640899poster.pdf)



QUANTITATIVE APPROACHES TO BIOMEDICAL BIG DATA

- QUBBD SUPPORTS RESEARCH AT THE INTERSECTION OF THE BIOMEDICAL AND DATA SCIENCES BY ENCOURAGING INTER- AND MULTI-DISCIPLINARY COLLABORATION
- 1 AWARD BY NSF (UP TO 2 MORE IN FY18) AND 7 BY NIH, TOTAL \$8.5M
- NEW NSF/DMS AND NATIONAL LIBRARY OF MEDICINE MOU FOR QUANTITATIVE DATA SCIENCE APPROACHES TO BIOMEDICAL DATA (FY2019)

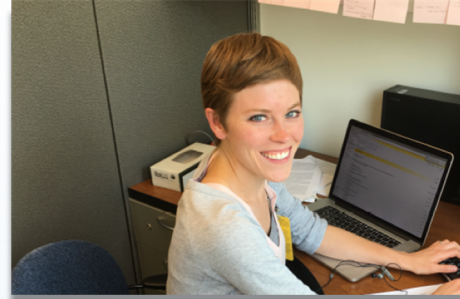


PERSISTENT HOMOLOGY USED TO DEVELOP QUANTITATIVE MORPHOLOGICAL DESCRIPTORS THAT CAPTURE ARCHITECTURAL FEATURES OF PROSTATE GLANDS IN PATHOLOGY IMAGES, WENK, DMS 1664848



MATHEMATICAL SCIENCES GRADUATE INTERNSHIP

- PROVIDE AN OPPORTUNITY FOR MATHEMATICAL SCIENCES DOCTORAL STUDENTS TO PARTICIPATE IN INTERNSHIPS AT NATIONAL LABORATORIES, INDUSTRY AND OTHER APPROVED FACILITIES
- AIMED AT STUDENTS WHO ARE INTERESTED IN UNDERSTANDING THE APPLICATION OF ADVANCED MATHEMATICAL AND STATISTICAL TECHNIQUES TO "REAL WORLD" PROBLEMS, REGARDLESS OF WHETHER THE STUDENT PLANS TO PURSUE AN ACADEMIC OR NONACADEMIC CAREER
- 40 GRADUATE STUDENTS FROM 38 UNIVERSITIES WORKED IN 10 NATIONAL LABS IN THE SUMMER OF 2017



SIAM News Article
(12/01/2017)

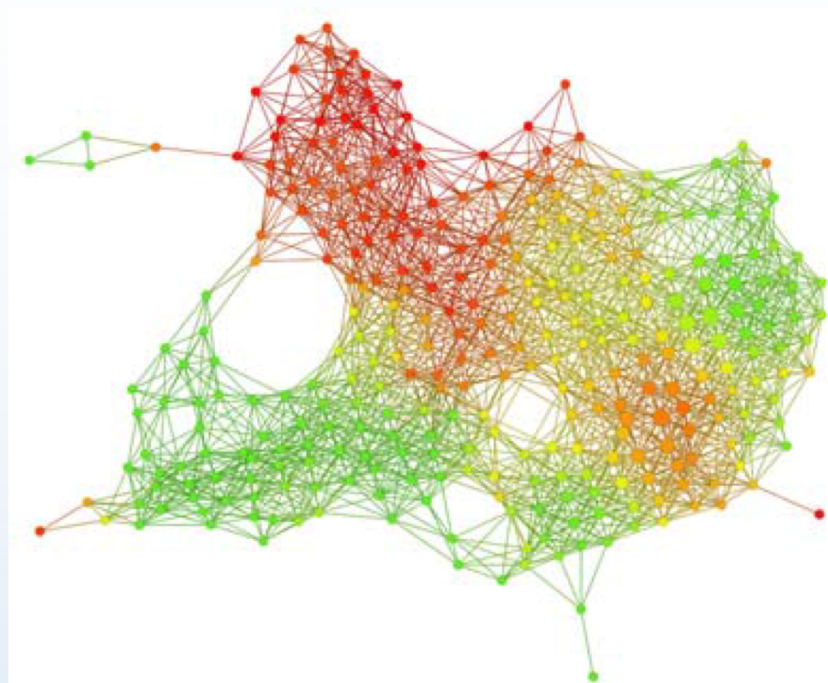


Managed by Oak Ridge Institute for Science and Education

Division of Mathematical Sciences

ON THE HORIZON – EXPANSION OF TRIPODS

- **TRIPODS+X:** Partnerships between SCI/ENG Fields and TRIPODS Institutes (NSF 18-542)
- Three tracks: Research, Visioning, and Education
- TRIPODS Phase II in FY 2020, anticipated to call for larger Institutes for up to 5 years of funding



Topological view of CT slices for traumatic brain injury. Red nodes represent slices with intracerebral hemorrhage, while green nodes show normal features. Brock, Brown University, CCF-1740741

THANK YOU

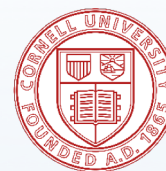


EXTRA SLIDES

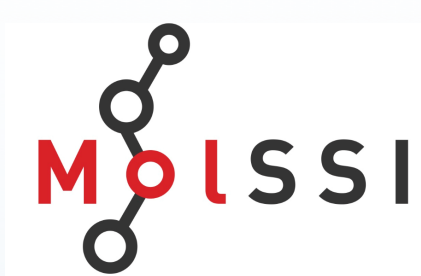


TRIPODS - TRANSDISCIPLINARY RESEARCH IN PRINCIPLES OF DATA SCIENCE

- Joint DMS & Division of Computing and Communications Foundations
- Bring together the statistics, mathematics, and theoretical computer science communities to develop the theoretical foundations of data science through integrated research and training activities
- 12 phase I awards. Each \$500K per year for three years
- First PI Meeting held in Oct. 2017



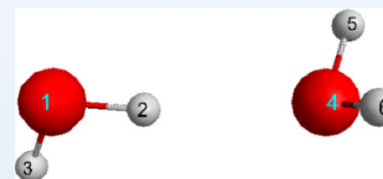
Cyberinfrastructure Investment in CHE:



<http://molssi.org/>

Molecular Sciences Software Institute — serving as a nexus for science, education, and cooperation for the community of computational molecular scientists (NSF 1547580, Daniel Crawford/Virginia Tech, supported by OAC/CHE/DMR)

SI2-SSI: Removing Bottlenecks in High Performance Computational Science — providing an integrated computational science approach to high quality electronic structure and dynamics calculation (NSF1450217, Mark Gordon/Iowa State U, supported by OAC/CHE/EPSCoR).



Water dimer optimized at the MP2/aug-cc-pVDZ level of theory.

J. Phys. Chem. A 2017, 121, 3736-3745.

